

WHAT IS CLAIMED IS:

- 1 1. A method for preparing a library of compounds, comprising:
 - 2 a) providing a plurality of individual synthesis templates each comprising a solid
 - 3 support, wherein said solid support has an interior portion and an exterior
 - 4 portion each with a plurality of reactive functional groups, wherein said solid
 - 5 support is linked to a scaffold via a scaffold linker, wherein said scaffold has
 - 6 at least two scaffold functional groups, and wherein at least two coding tag
 - 7 precursors, each comprising a coding functional group and a coding linker, are
 - 8 attached to said solid support;
 - 9 b) contacting a first synthesis template with a first reactive component such that a
 - 10 first scaffold functional group reacts with said first reactive component to
 - 11 afford a first scaffold building block, and a first coding functional group reacts
 - 12 with said first reactive component to afford a first coding building block;
 - 13 c) contacting said first synthesis template with a successive reactive component such
 - 14 that a subsequent scaffold functional group reacts with said successive reactive
 - 15 component to afford a subsequent scaffold building block, and a subsequent
 - 16 coding functional group reacts with said successive reactive component to
 - 17 afford a subsequent coding building block;
 - 18 d) repeating step c) until said first compound has been prepared; and
 - 19 e) subjecting additional synthesis templates to steps b) - d) with additional reactive
 - 20 components to prepare said library of compounds.
- 1 2. The method of claim 1, further comprising the following step:
 - 2 f) cleaving each of said compounds from each of said synthesis templates.

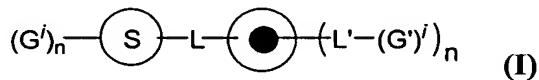
- 1 3. The method of claim 1, wherein the number of said scaffold functional
- 2 groups equals the number of said coding functional groups.

- 1 4. The method of claim 1, wherein said reactive component reacts with
- 2 said scaffold functional group and said coding functional group via a reaction selected from
- 3 the group consisting of amine acylation, reductive alkylation, aromatic reduction, aromatic
- 4 acylation, aromatic cyclization, aryl-aryl coupling, [3+2] cycloaddition, Mitsunobu reaction,
- 5 nucleophilic aromatic substitution, sulfonylation, aromatic halide displacement, Michael
- 6 addition, Wittig reaction, Knoevenagel condensation, reductive amination, Heck reaction,

7 Stille reaction, Suzuki reaction, Aldol condensation, Claisen condensation, amino acid
8 coupling, amide bond formation, acetal formation, Diels-Alder reaction, [2+2] cycloaddition,
9 enamine formation, esterification, Friedel Crafts reaction, glycosylation, Grignard reaction,
10 Horner-Emmons reaction, hydrolysis, imine formation, metathesis reaction, nucleophilic
11 substitution, oxidation, Pictet-Spengler reaction, Sonogashira reaction, thiazolidine
12 formation, thiourea formation and urea formation.

1 5. The method of claim 1, wherein said compounds of said library are
2 prepared in parallel.

1 6. The method of claim 1, wherein at least one of said synthesis templates
2 has a structure of formula I:



4 wherein

5 $(G^i)_n$ represents n independent scaffold functional groups, G^i to G^n , wherein each G^i is
6 one of said scaffold functional groups;

7  is said scaffold;

8 L is said scaffold linker;

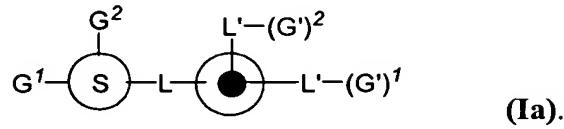
9  is said solid support, wherein the darkened portion represents said interior
10 portion of said solid support, and the lightened portion represents said exterior
11 portion of said solid support;

12 $(-L' - (G')^i)_n$ represents n independent coding tag precursors, wherein each of said
13 coding tag precursors comprises one of n independent coding functional
14 groups, $(G')^i$ to $(G')^n$, each linked to said solid support via one of n coding
15 linkers, wherein each $(G')^i$ is one of said coding functional groups, and L' is
16 said coding linker;

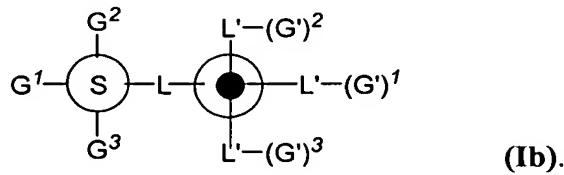
17 subscript n is an integer from 2 to 10; and

18 superscript i is an integer from 1 to n.

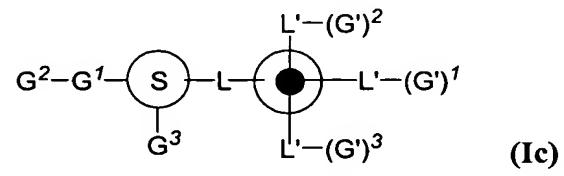
1 7. The method of claim 6, wherein said synthesis template has a structure
2 of formula Ia:



1 8. The method of claim 6, wherein said synthesis template has a structure
2 of formula Ib:



1 9. The method of claim 1, wherein said synthesis template has a structure
2 of formula Ic:



4 wherein

5 each of G', G² and G³ is one of said scaffold functional groups;

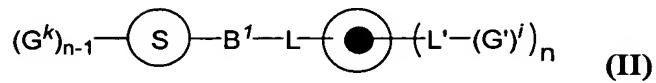
6 is said scaffold;

7 L is said scaffold linker;

8 is said solid support, wherein the darkened portion represents said interior
9 portion of said solid support, and the lightened portion represents said exterior
10 portion of said solid support; and

11 each of -L'-(G')¹, -L'-(G')² and -L'-(G')³ is one of said coding tag precursors, each
12 comprising said coding functional group linked to said solid support via said
13 coding linker.

1 10. The method of claim 1, wherein at least one of said synthesis templates
2 has a structure of formula II:



4 wherein

5 B^1 represents a first scaffold building block;

6 $(G^k)_{n-1}$ represents $n-1$ independent scaffold functional groups, G^2 to G^n , wherein each
7 G^k is one of said scaffold functional groups;

8 \textcircled{S} is said scaffold;

9 L is said scaffold linker;

10 $\textcircled{\bullet}$ is said solid support, wherein the darkened portion represents said interior
11 portion of said solid support, and the lightened portion represents said exterior
12 portion of said solid support;

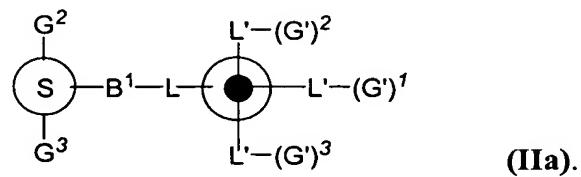
13 $(-L' - (G')^i)_n$ represents n independent coding tag precursors, wherein each of said
14 coding tag precursors comprises one of n independent coding functional
15 groups, $(G')^1$ to $(G')^n$, each linked to said solid support via one of n coding
16 linkers, wherein each $(G')^i$ is one of said coding functional groups, and L' is
17 said coding linker;

18 subscript n is an integer from 2 to 10;

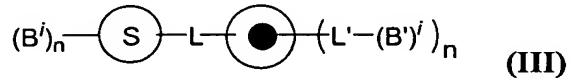
19 superscript i is an integer from 1 to n ; and

20 superscript k is an integer from 2 to n .

1 11. The method of claim 10, wherein said synthesis template has a
2 structure of formula IIa:



1 12. The method of claim 1, wherein said steps a) - d) afford a compound
2 template of formula III:



4 wherein

5 $(B^i)_n$ represents n independent scaffold building blocks, B^1 to B^n , wherein each B^i is
6 one of said scaffold building blocks;

7  is said scaffold;

8 L is said scaffold linker;

9  is said solid support, wherein the darkened portion represents said interior
10 portion of said solid support, and the lightened portion represents said exterior
11 portion of said solid support;

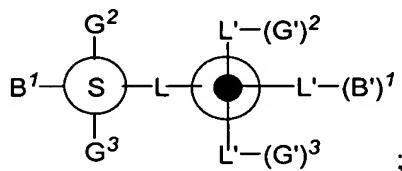
12 $(-L'-(B')^i)_n$ represents n independent coding tags, wherein each of said coding tags
13 comprises one of n independent coding building blocks, $(B')^1$ to $(B')^n$, each
14 linked to said solid support via one of n coding linkers, wherein each $(B')^i$ is
15 one of said coding building blocks, and L' is said coding linker;

16 subscript n is an integer from 2 to 10; and

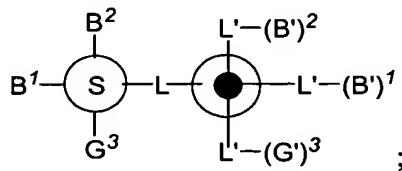
17 superscript i is an integer from 1 to n.

1 13. The method of claim 1, comprising:

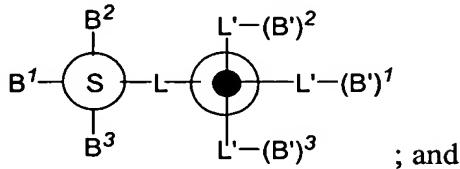
2 a) providing a plurality of individual synthesis templates according to formula Ib;
3 b) contacting a first synthesis template with a first reactive component to afford the
4 following structure:



5 c) contacting said first synthesis template with a successive reactive component to
6 afford the following structure:



9 d) repeating step c) to prepare said compound attached to the following compound
10 template according to claim 12:



12 e) subjecting additional of said synthesis templates to steps b) - d) with additional of
13 said reactive components in order to prepare said library of compounds.

1 14. The method of claim 13, further comprising the following step:

2 f) cleaving each of said compounds from each of said compound templates.

1 15. The method of claim 1, wherein, on each of said synthesis templates,
2 each of said scaffold building blocks is encoded by a single coding building block.

1 16. The method of claim 1, further comprising the following step:

2 f) decoding each of said compounds by cleaving each of said coding tags from said
3 synthesis template and analyzing said coding tags to determine the identity of
4 said corresponding scaffold building blocks.

1 17. The method of claim 17, wherein said analyzing is carried out via mass
2 spectrometry.

1 18. The method of claim 1, wherein said scaffold is the same on each of
2 said synthesis templates.

1 19. The method of claim 1, wherein at least two different scaffolds are
2 used.

1 20. The method of claim 1, wherein said scaffold is a member selected
2 from the group consisting of quinazoline, tricyclic quinazoline, purine, pyrimidine,
3 phenylamine-pyrimidine, phthalazine, benzylidene malononitrile, amino acid, tertiary amine,
4 peptide, lactam, sultam, lactone, pyrrole, pyrrolidine, pyrrolinone, oxazole, isoxazole,
5 oxazoline, isoxazoline, oxazolinone, isoxazolinone, thiazole, thiazolidinone, hydantoin,
6 pyrazole, pyrazoline, pyrazolone, imidazole, imidazolidine, imidazolone, triazole,
7 thiadiazole, oxadiazole, benzofuran, isobenzofuran, dihydrobenzofuran,
8 dihydroisobenzofuran, indole, indoline, benzoxazole, oxindole, indolizine, benzimidazole,

9 benzimidazolone, pyridine, piperidine, piperidinone, pyrimidinone, piperazine, piperazinone,
10 diketopiperazine, metathiazanone, morpholine, thiomorpholine, phenol, dihydropyran,
11 quinoline, isoquinoline, quinolinone, isoquinolinone, quinolone, quinazolinone,
12 quinoxalinone, benzopiperazinone, quinazolinedione, benzazepine and azepine.

1 21. The method of claim 1, wherein said library of compounds is prepared
2 via a split-mix methodology.

1 22. A library of compounds prepared by the method of claim 1.

1 23. A library of compounds prepared by the method of claim 2.

1 24. A method for identifying a compound of claim 1 that binds to a target,
2 said method comprising:

3 a) contacting said compound of claim 1 with said target; and
4 b) determining the functional effect of said compound upon said target.

1 25. The method of claim 24, wherein said biological target is a protein
2 kinase.

1 26. A method for identifying a compound of claim 2 that binds to a target,
2 said method comprising:

3 a) contacting said compound of claim 2 with said target; and
4 b) determining the functional effect of said compound upon said target.

1 27. The method of claim 26, wherein said target is a protein kinase.

1 28. A method for preparing a library of compounds, comprising:

2 a) providing a population of individual synthesis templates each comprising a solid
3 support, wherein said solid support has an interior portion and an exterior
4 portion each with a plurality of reactive functional groups, wherein said solid
5 support is linked to a scaffold via a scaffold linker, wherein said scaffold has
6 at least two scaffold functional groups, and wherein at least two coding tag
7 precursors, each comprising a coding functional group and a coding linker, are
8 attached to said solid support;
9 b) splitting said population of synthesis templates into two or more separate pools;

10 c) contacting said population of synthesis templates with one or more first reactive
11 components in said two or more separate pools such that a first scaffold
12 functional group reacts with one of said first reactive components to afford a
13 first scaffold building block, and a first coding functional group reacts with
14 one of said first reactive components to afford a first coding building block,
15 wherein said contacting step yields subsequent synthesis templates;
16 d) mixing said subsequent synthesis templates from said two or more separate pools
17 into a single pool;
18 e) splitting said subsequent synthesis templates into two or more separate pools;
19 f) contacting said subsequent synthesis templates in said two or more separate pools
20 with a successive reactive component such that a subsequent scaffold
21 functional group reacts with said successive reactive component to afford a
22 subsequent scaffold building block, and a subsequent coding functional group
23 reacts with said successive reactive component to afford a subsequent coding
24 building block, wherein said contacting step yields further synthesis templates;
25 g) repeating steps d) - f), wherein said further synthesis templates of step f) become
26 said subsequent synthesis templates of step d), until said library of compounds
27 has been prepared.